MAX PLANCK GESELLSCHAFT

MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

Bridging continuous and discrete tensor representations of multivariate functions via QTT

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Based on a joint work with
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Partners:

MAX PLANCK INSTITUTE
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Organization

Discrete and continuous tensor formats

Consider $f : [-1, 1]^D \to \mathbb{R}$, $D = 3$. Approx. f with a *small number of parameters* $\rightsquigarrow$ cheap comput. with f.

1. **Grid-based methods**: discrete Tucker format of function related tensor $\mathbf{F}$ (contains, e.g., function values on a grid):

$$\mathbf{F}(i_1, i_2, i_3) \approx \sum_{j_1=1}^{R} \sum_{j_2=1}^{R} \sum_{j_3=1}^{R} \boldsymbol{\beta}_{j_1,j_2,j_3} \mathbf{u}_{j_1}^{(1)}(i_1) \mathbf{u}_{j_2}^{(2)}(i_2) \mathbf{u}_{j_3}^{(3)}(i_3), \mathbf{u}_{j_\ell}^{(\ell)} \in \mathbb{R}^n, \ \mathbf{F} \in \mathbb{R}^{n\times n\times n}.$$

2. **Mesh-free methods**: functional Tucker format of f:

$$f(x_1, x_2, x_3) \approx f_{\mathbf{m}}(x_1, x_2, x_3) := \sum_{i_1=1}^{R} \sum_{i_2=1}^{R} \sum_{i_3=1}^{R} \boldsymbol{\beta}_{i_1,i_2,i_3} v_{i_1}^{(1)}(x_1) v_{i_2}^{(2)}(x_2) v_{i_3}^{(3)}(x_3) \tag{1}$$

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We call Eq. (1) the **Chebyshev-Tucker (ChebTuck) format**.

ChebTuck to Grid-based tensor

- Consider $f : [-1, 1]^3 \to \mathbb{R}$ approximated in **ChebTuck format**:

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with $v_{i_\ell}^{(\ell)}(x_\ell) = \sum_{j_\ell=1}^{m} V_{j_\ell,i_\ell}^{(\ell)} T_{j_\ell-1}(x_\ell),\ T_{j_\ell}(x) = \cos(j_\ell \arccos(x))$. **Storage**: $\mathcal{O}(DRm + R^D)$.

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- **Goal**: Transform ChebTuck format to a discrete tensor format on a fine grid $n \gg m$:

$$\mathbf{F}_{\mathbf{m}}(i_1,i_2,i_3) := f_{\mathbf{m}}(t_{i_1}^{(1)}, t_{i_2}^{(2)}, t_{i_3}^{(3)}), \quad \{t_{i_\ell}^{(\ell)}\}_{i_\ell=1}^{n} \text{ is a uniform grid in } [-1,1].$$

- **Motivation**:
  - Efficient application of discrete operators (differentiation, integration, convolution).
  - Offline-online workflows: expensive offline construction of continuous surrogate, fast online evaluation.
  - High-resolution discretizations for accurate simulations.

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- The **naive approach** yields a discrete Tucker:

$$\mathbf{F}_{\mathbf{m}} = \boldsymbol{\beta} \times_1 U_1 \times_2 U_2 \times_3 U_3, \quad U_\ell(i_\ell, j_\ell) = v_{j_\ell}^{(\ell)}(t_{i_\ell}^{(\ell)})$$

  i.e., each column of U_ℓ contains the discretization of a Chebyshev poly. $v_{j_\ell}^{(\ell)}(x_\ell)$ on the grid $t_{i_\ell}^{(\ell)}$.

- **Storage**: $\mathcal{O}(DRn + R^D)$. **Additional storage** compared to ChebTuck: $\mathcal{O}(DRn)$, $n \gg m$.

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- **Remedy:** store columns of U_ℓ as quantized tensor trains (QTT) [Khoromskij '11].
- **QTT**: a vector $\mathbf{u} \in \mathbb{R}^n$ with $n = 2^d$, reshape $\mathbf{u}$ to a d-dimensional tensor $\mathbf{U} \in \mathbb{R}^{2\times\cdots\times 2}$ and approximate $\mathbf{U}$ in TT format: $\mathbf{U}(i_1,\ldots,i_d) = \mathbf{G}_1(i_1)\mathbf{G}_2(i_2)\cdots\mathbf{G}_d(i_d)$ for $i_1,\ldots,i_d = 0,1$.
  Storage: $r^2 d = \mathcal{O}(r^2 \log n)$, where r is the TT rank.

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- Known: QTT ranks of polynomials p of degree m are bounded by $m+1$ [Khoromskij '11, Oseledets '13] (numerically even $\log m$) $\rightsquigarrow$ $\mathcal{O}(DRn)$ reduced to $\mathcal{O}(DRm^2 \log n)$ (numerically $\mathcal{O}(DR \log^2 m \log n)$).

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- **Fundamental task**: approximate a polynomial p in QTT format efficiently.

From ChebTuck to QTT-Tucker

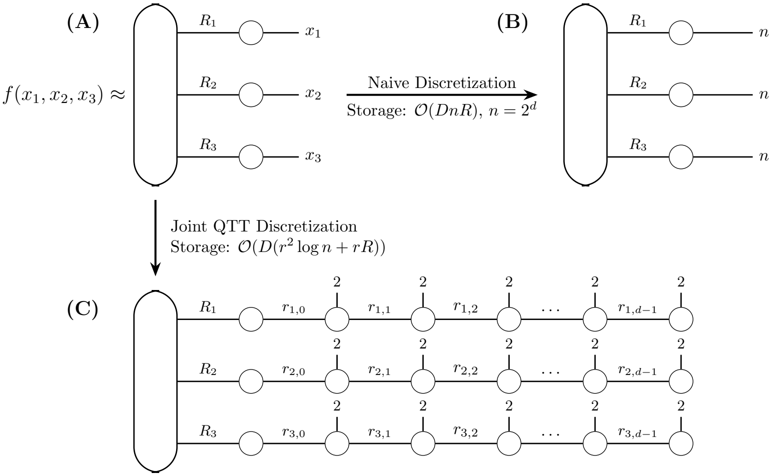

Figure: (A) Continuous ChebTuck. (B) Discrete Tucker ($\mathcal{O}(n)$ storage). (C) QTT-Tucker-like ($\mathcal{O}(\log n)$ storage).

Organization

Approximation of a polynomial in QTT format

- For a polynomial $p(x) = p_0 + p_1 x + \cdots + p_m x^m$ in $[-1, 1]$, discretizing it on uniform grid $\{x_i := -1 + ih\}_{i=0}^{n-1}$ with $h = 2/n$ and $n = 2^d$ yields $\mathbf{p} = \{p(x_i)\}_{i=1}^{n} \in \mathbb{R}^{2^d}$.

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- Use the multi-index mapping $(i_1, \ldots, i_d) \mapsto i = i_1 + 2 \cdot i_2 + \cdots + 2^{d-1} \cdot i_d$ for $i_\ell = 0, 1$
- Reshape $\mathbf{p}$ to a d-dimensional tensor $\mathbf{P} \in \mathbb{R}^{2 \times \cdots \times 2}$:

$$\mathbf{P}(i_1, \ldots, i_d) = p(x_i) = p\Big(- 1 + i_1 h + 2 \cdot i_2 h + \cdots + 2^{d-1} \cdot i_d h\Big)$$

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\begin{aligned}
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Computational methods for the TT of P

1. **Direct method**: apply directly the adaptive TT cross, e.g., `dmrg_cross` [Savostyanov/Oseledets '11].
2. **Constructive method**: there exists an analytic formula[1] for the cores $\mathbf{G}_\ell(i_\ell) \in \mathbb{R}^{(m+1)\times(m+1)}$.

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Disadvantages: Method 1 does not exploit the 1D nature of the problem, just views $\mathbf{P}$ as a black box tensor. Method 2 quickly becomes numerically unstable & produces pessimistic TT ranks $m + 1$.

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3. **Our novel method**: Constructive (thus faster than Method 1), stable and rank adaptive.

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Recall Oseledets' constructive method

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Fix: replace x^α, y^β by Chebyshev poly.: $p(x+y) = \sum_{\alpha=0}^{m}\sum_{\beta=0}^{m} M_m^{\mathrm{cheb}}(\alpha,\beta) T_\alpha(x) T_\beta(y)$.

Direct construction in Chebyshev basis

Fix: Replace monomial expansion

$$p(x+y) = \sum_{\alpha=0}^{m} \sum_{\beta=0}^{m} M(\alpha, \beta) x^{\alpha} y^{\beta} \tag{2}$$

by Chebyshev expansion

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- **Subtle but crucial difference**:
  - (2) holds for all $x, y \in \mathbb{R}$ for fixed M
  - (3) only holds for $x \in I_x$ and $y \in I_y$ with some intervals I_x, I_y and M_m^{cheb} depend accordingly on these intervals.
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  - Algorithmically: carefully track the intervals I_x, I_y the auxiliary variables $x_{i_\ell}^{(\ell)}$ live in during the construction.
- **Rank-adaptivity**: apply truncated SVDs on the fly.

Rank-adaptive construction (Error control)

- All SVD tolerances during the process are chosen as ε.
- We have guaranteed element-wise error control.

Theorem [Benner, Khoromskij, S., in preparation, 2026]

For the QTT approximation of the polynomial $p(x)$ constructed by the rank-adaptive method, we have

$$|\mathbf{P} - \hat{\mathbf{P}}| \leq (\sqrt{m+1} + 1)(d-1)\varepsilon$$

Organization

1. Introduction
2. QTT approximation of polynomials
3. Fully discrete format
4. Numerical experiments
5. Conclusion

ChebTuck to Grid-based tensor

- Consider $f : [-1,1]^3 \to \mathbb{R}$ approximated in **ChebTuck format**:

$$f(x_1, x_2, x_3) \approx f_{\mathbf{m}}(x_1, x_2, x_3) = \sum_{i_1=1}^{R} \sum_{i_2=1}^{R} \sum_{i_3=1}^{R} \boldsymbol{\beta}_{i_1,i_2,i_3} v_{i_1}^{(1)}(x_1) v_{i_2}^{(2)}(x_2) v_{i_3}^{(3)}(x_3),$$

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- **Goal**: Transform ChebTuck format to a discrete tensor format on a fine grid $n \gg m$:

$$\mathbf{F}_{\mathbf{m}}(i_1,i_2,i_3) := f_{\mathbf{m}}(t_{i_1}^{(1)}, t_{i_2}^{(2)}, t_{i_3}^{(3)}), \quad \{t_{i_\ell}^{(\ell)}\}_{i_\ell=1}^{n} \text{ is a uniform grid in } [-1,1].$$

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- Apply our QTT approximation algorithm to each polynomial $v_{j_\ell}^{(\ell)}(x_\ell)$.

From ChebTuck to QTT-Tucker

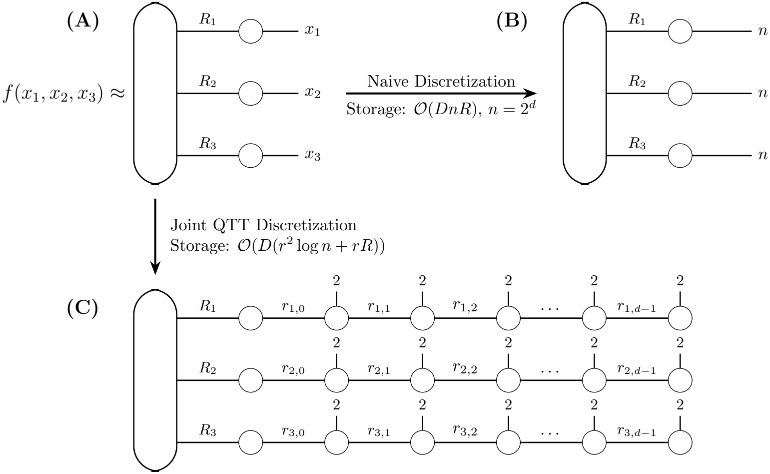

Figure: (A) Continuous ChebTuck. (B) Discrete Tucker ($\mathcal{O}(n)$ storage). (C) QTT-Tucker-like ($\mathcal{O}(\log n)$ storage).

Organization

Random polynomials in monomial basis

- Non-trivial, but practical and not pathological (not too oscillatory) polynomials.
- Polynomials of degree m (up to 300) with random coefficients:

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m.$$

- a_k decays exponentially with random relative noise.
- Discretization on uniform grid with $n = 2^{20}$ points (20 dimensional QTT tensor).
- Tolerances of all SVDs in our method are set to 10^{-12}.
- `dmrg_cross` tolerance is set to 10^{-12}.

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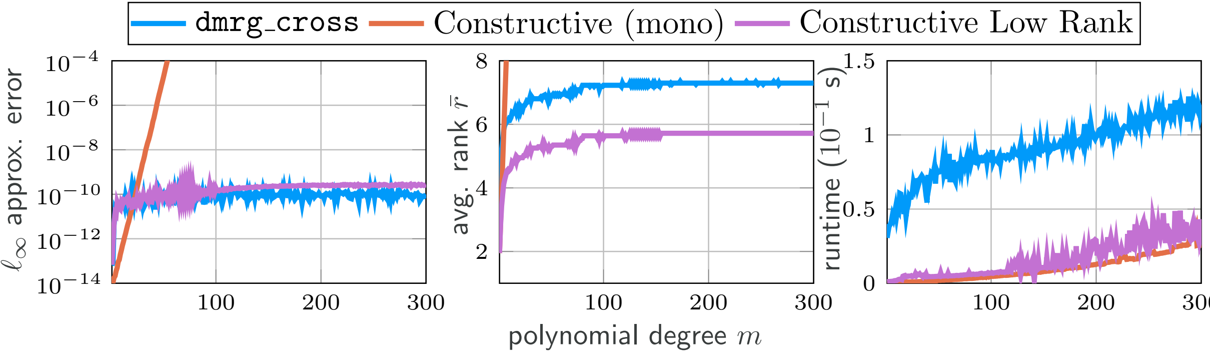

Random polynomials in Chebyshev basis

- Chebyshev polynomials of degree m (up to 300) with random coefficients:

$$p(x) = a_0 + a_1 T_1(x) + a_2 T_2(x) + \cdots + a_m T_m(x).$$

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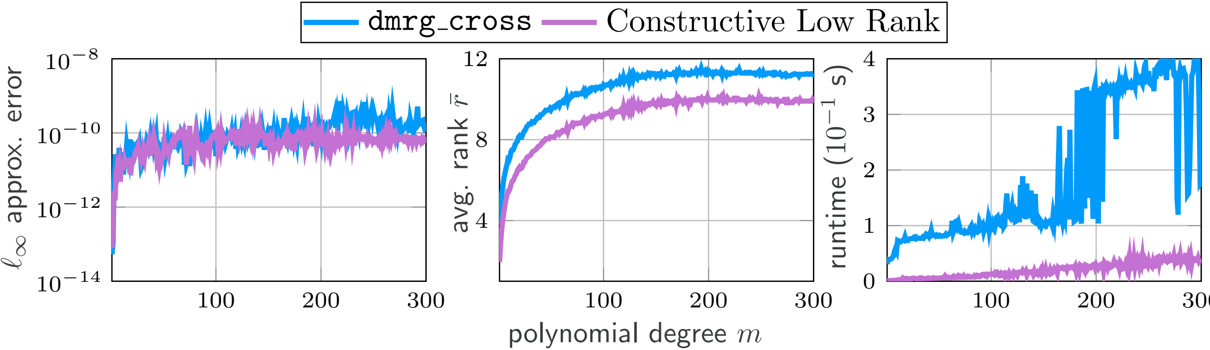

Single Chebyshev polynomials

- A single Chebyshev polynomial $T_m(x)$ of degree m (up to 300).
- Very challenging since it is highly oscillatory.

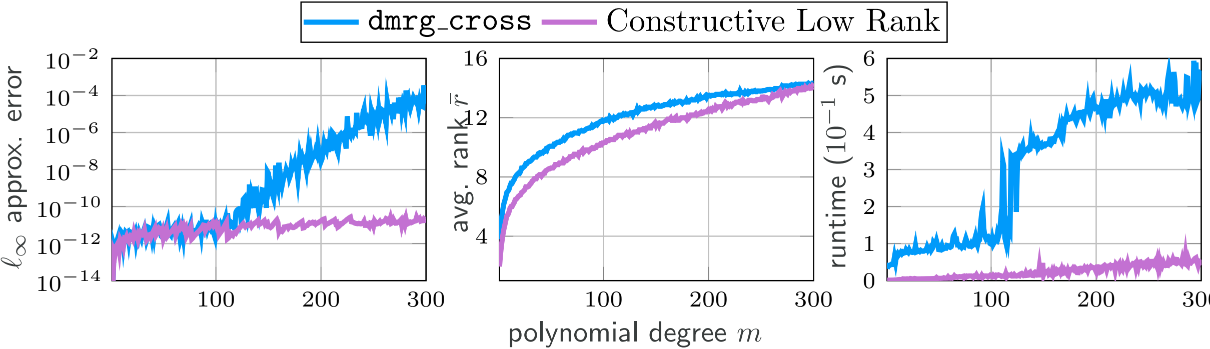

Figure: TTCross vs. Constructive Low Rank.

Test functions

We consider the following 3 test functions $f : [-1, 1]^3 \to \mathbb{R}$:

1. **Biomolecule potential** f_1: the multi-particle potential of the protein Fasciculin 1 comprising 1,228 atoms[2].
2. **Runge function** f_2: the classical 3-dimensional Runge function[3] given by

$$f_2(x, y, z) = \frac{1}{1 + 25(x^2 + y^2 + z^2)}. \tag{4}$$

3. **Wagon function** f_3: the SIAM 100-Dollar, 100-Digit Challenge function[4] defined by

$$\begin{aligned} f_3(x, y, z) = {} & e^{\sin(50x)} + \sin(60e^y)\sin(60z) + \sin(70\sin(x))\cos(10z) \\ & + \sin(\sin(80y)) - \sin(10(x+z)) + \frac{x^2 + y^2 + z^2}{4}. \end{aligned} \tag{5}$$

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[2] M.H. Le Du, P. Marchot, P.E. Bougis, and J.C. Fontecilla-Camps, J. Biol. Chem., 267:22122–30, 1992.
[3] B. Hashemi and L. N. Trefethen, SIAM J. Sci. Comput., 39(5):C341–C363, 2017.
[4] F. Bornemann, D. Laurie, S. Wagon, and J. Waldvogel. SIAM, 2004.

- Combining ChebTuck

$$f(x_1, x_2, x_3) \approx \sum_{i_1=1}^{R} \sum_{i_2=1}^{R} \sum_{i_3=1}^{R} \beta_{i_1,i_2,i_3} v_{i_1}^{(1)}(x_1) v_{i_2}^{(2)}(x_2) v_{i_3}^{(3)}(x_3),$$

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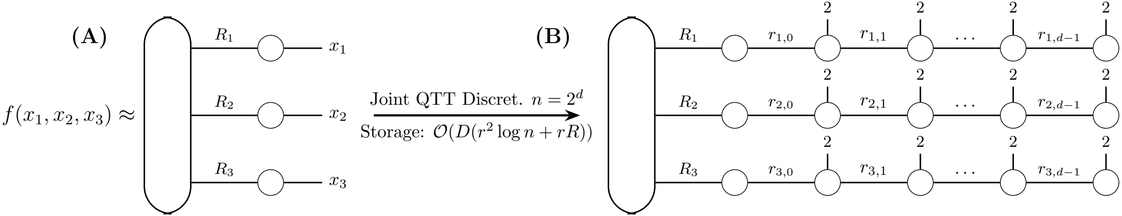
$$\mathbf{F}(i_1, i_2, i_3) \approx \boldsymbol{\beta} \times_1 \mathbf{U}^{(1)}(i_1) \times_2 \mathbf{U}^{(2)}(i_2) \times_3 \mathbf{U}^{(3)}(i_3).$$



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Function	**Tucker ranks**	**Polynomial degrees**
f_1	(32, 28, 32)	(129, 129, 129)
f_2	(17, 17, 17)	(189, 189, 189)
f_3	(4, 3, 5)	(662, 1052, 129)

Joint QTT approximation of multiple polynomials

function	method	ℓ_∞ error	storage	avg. rank $\bar{r}$	runtime (10^{-1} s)
f_1	**Constructive Low Rank**	$\mathbf{5.12 \times 10^{-11}}$	**20,550**	21.60	**0.4**
	`dmrg_cross`	7.30×10^{0}	7,770	13.01	5.6
f_2	**Constructive Low Rank**	$\mathbf{1.82 \times 10^{-11}}$	**4,875**	10.49	**0.2**
	`dmrg_cross`	4.15×10^{-8}	5,317	10.98	5.0
f_3	**Constructive Low Rank**	$\mathbf{3.10 \times 10^{-9}}$	**4,182**	9.97	**1.5**
	`dmrg_cross`	4.23×10^{-8}	5,342	11.27	7.1

Table: ChebTuck factors from biomolecule f_1, Runge f_2, and wagon f_3; $n = 2^{20}$.

Fully discrete QTT–Tucker format

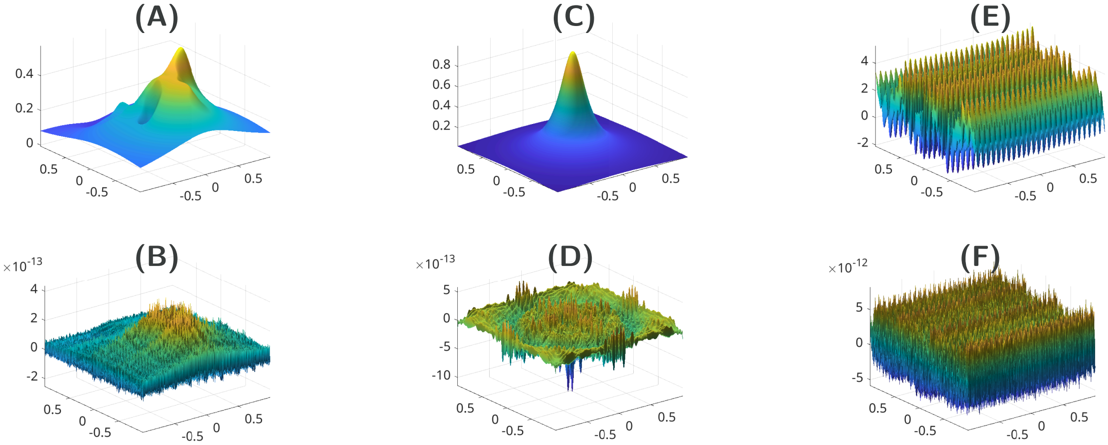

Figure: **(A)**, **(C)**, **(E)**: Surfaces reconstructed from the fully discrete QTT-Tucker format for $f_i(x, y, 0)$.
(B), **(D)**, **(F)**: Corresponding pointwise errors compared to the continuous tensors.

Conclusion

- A framework to bridge continuous and discrete tensor formats via QTT.
- Developed stable and rank-adaptive algorithms for QTT approximation of polynomials.
- Numerical experiments demonstrate stability, efficiency, and storage savings.
- **Outlook**: Extend it to general univariate functions and multivariate ridge functions and more application scenarios.
- For more details and reference:

1. P. Benner, B. Khoromskij, B. Sun. *Bridging continuous and discrete tensor representations of multivariate functions using QTT*, in preparation, 2026.
2. P. Benner, B. Khoromskij, V. Khoromskaia, B. Sun. *A mesh-free hybrid Chebyshev-Tucker tensor format with applications to multi-particle modelling*, arXiv:2505.02319, 2025.

Thank you for your attention!